Linear Regression Sand Box and Open Hand Problem

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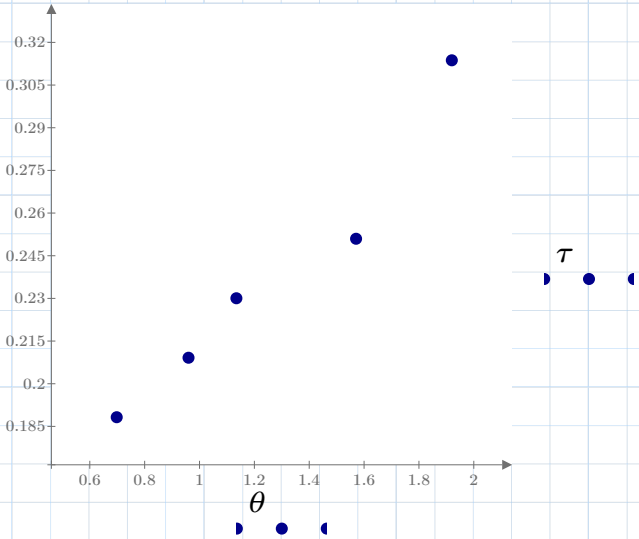
θ	τ
0.698132	0.188224
0.959931	0.209138
1.134464	0.230052
1.570796	0.250965
1.919862	0.313707

To the left is a dataset from Kau's NM-MFC 06.03's Example 1 where we are playing with mousetraps...

Let's use this case to explore basic linear regression theory and execution. We can also take this example to illustrate how linear regression, correlation and predictive skill are related.

First, let's plot these two fields against each other...



It clearly makes a nice linear relationship.

Let's now pull some basic stats...

$$\theta_{mean} := \text{mean}(\theta) = 1.257$$
$$s_\theta := \text{Stdev}(\theta) = 0.488$$
$$\tau_{mean} := \text{mean}(\tau) = 0.238$$
$$s_\tau := \text{Stdev}(\tau) = 0.048$$
$$N := \text{rows}(\theta) = 5$$
$$\alpha := 100\% - 95\% = 0.05$$

$$CI95_\theta := \text{qt}\left(1 - \frac{\alpha}{2}, N-1\right) \cdot \frac{s_\theta}{\sqrt{N}} = 0.606$$

$$CI95_\tau := \text{qt}\left(1 - \frac{\alpha}{2}, N-1\right) \cdot \frac{s_\tau}{\sqrt{N}} = 0.06$$

We will be creating a function to fit the dependent variable τ to independant variable θ

$$\tau_\theta(\theta) = a_0 + a_1 \cdot \theta$$

Remember the secret to linear regression. We want to minimize the error between our regression equation results and our original values of tau. We express it as a summed square of the residuals (SSR) or Sr. We can also express this as a "Cost" or "Error" function if we were to look at this problem from a very general sense.

$$S_r(a_0, a_1) := \sum \left(\left((a_0 + a_1 \cdot \theta) - \tau \right)^2 \right)$$

If we were to take our values of tau and theta up top and plug them into the above equation (and shrink the font down to microscopic scale so we can see the whole thing) we get the following polynomial function for which we now must solve for a0 and a1

$$S_r(a_0, a_1) \xrightarrow{simplify} 5.0 \cdot {a_0}^2 + 12.56637 \cdot a_0 \cdot a_1 - 2.384172 \cdot a_0 + 8.849134554141 \cdot {a_1}^2 - 3.179275851496 \cdot a_1 + 0.293486412998$$

Put in other words we need to ***calibrate*** our values of a0 (y-intercept) and a1 (slope) to minimize the error that is crunched by the formula above.

So how do we do this in a way that is efficient, accurate and mathematically sound?

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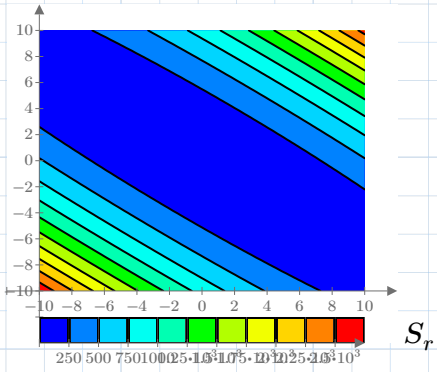
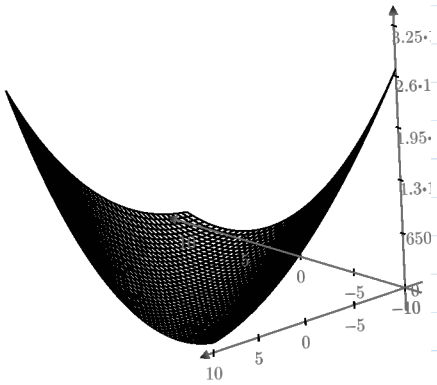
$$S_r(a_0, a_1) \xrightarrow{simplify} 5.0 \cdot a_0^{\,2} + 12.56637 \cdot a_0 \cdot a_1 - 2.384172 \cdot a_0 + 8.849134554141 \cdot a_1^{\,2} - 3.179275851496 \cdot a_1 + 0.293486412998$$

Here we are plotting Sr vs a0 and a1 in a contour plot

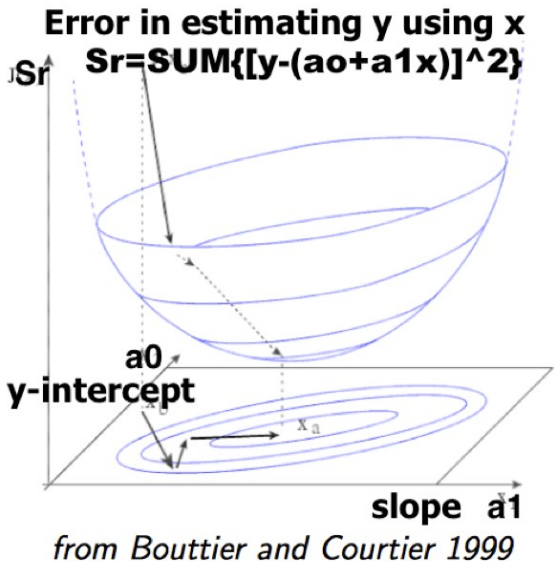
Somewhere is the blue is the minimum Sr.

Below is it plotted in 3D and to the side is an idealized version our error function.





$S_r(x, y)$



from Bouttier and Courtier 1999

x:a0, y-intercept
y:a1, slope
z: Sr/SSR/Error/Cost...

An idealization of a 2-D representation

If you remember your Calc-Fu there is a very straight forward to to do this. Our magic answer for our slope and intercept will be where the gradient (derivative) of our SSR/Sr/ Cost function is zero.

This method not only applies to linear regression but also to multivariate regression and many other types of calibration. Including those cases where we are calibrarting not just two parameters like slope and intercept, but 10s or even 100s of parameters.

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So let's take our Sr function and take the a0 (intercept) and a1 (slope) derivative of it.

$$S_r(a_0, a_1) \xrightarrow{simplify} 5.0 \cdot {a_0}^2 + 12.56637 \cdot a_0 \cdot a_1 - 2.384172 \cdot a_0 + 8.849134554141 \cdot {a_1}^2 - 3.179275851496 \cdot a_1 + 0.293486412998$$

So let's take our Sr function and take the a0 (intercept) and a1 (slope) derivative of it.

$$\frac{\mathrm{d}}{\mathrm{d}a_0} S_r(a_0, a_1) \rightarrow 10 \cdot a_0 + 12.56637 \cdot a_1 - 2.384172$$

$$\frac{\mathrm{d}}{\mathrm{d}a_1} S_r(a_0, a_1) \rightarrow 12.56637 \cdot a_0 + 17.698269108282 \cdot a_1 - 3.179275851496$$

So for our problem, our a0 (intercept) and a1 (slope) will be valid where both derivatives/slopes [or together, the "gradient"] are equal to zero.

$$\begin{bmatrix} \frac{\partial S_r(a_0, a_1)}{\partial a_0} \\ \frac{\partial S_r(a_0, a_1)}{\partial a_1} \end{bmatrix} = 0$$

Or if you've had vector Calc (in Calc 2 or Calc 3 depending on your college)

$$\vec{\nabla} S_r(\vec{a}) = 0$$

Where the vetor a represents ***all*** of the coefficients that you need to calibarate whether it's just
slope & intercept,
"slopes" for cement and water & "intercept"
1000 variables' "slopes" & "intercept"

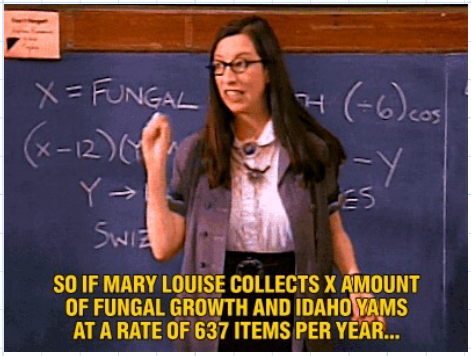
With respect to our problem, see just have to solve a0 and a1 for these two equations.

$$10 \cdot a_0 + 12.56637 \cdot a_1 - 2.384172 = 0$$
$$12.56637 \cdot a_0 + 17.698269108282 \cdot a_1 - 3.179275851496 = 0$$

So now our seemingly scary problem becomes an even scarier flashback to Junior High Algebra class with Mrs. Mercer.

This also becomes a blend of classic "root" or "zero" problem and linear algebra problem in Numerical Methods.

Either way, Mathcad acutally has several ways to attack this problem.



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For starters, let's just cut to the easy answers. There are established formulas for getting the slope and intercept for a two-variable calibration (which is what linear regression is)

$$slope\_c := \frac{N \cdot \sum_{i=0}^{N-1} \left(\theta_i \tau_i\right) - \sum \theta \cdot \sum \tau}{N \cdot \sum \theta^2 - \left(\sum \theta\right)^2} = 0.096 \qquad yint\_c := \tau_{mean} - slope\_c \cdot \theta_{mean} = 0.118$$

And with so many other frequently used operations, there are intrinsic functions to do this

$$A_1 := \text{slope}(\theta, \tau) = 0.096 \qquad A_0 := \text{intercept}(\theta, \tau) = 0.118$$

So far so good. Everything Matches!

But since this Sandbox is more than about just plugging and chugging.
Let's see what other tricks in Matchad we can use that may be useful in other problems

If you haven't been using units, the Maximum-Statisfaction-With-Minimal-Effort Tactic is to use the Sybolic Arrow with the Solve Command

$$\begin{bmatrix} \frac{d}{da_0} S_r(a_0, a_1) \\ \frac{d}{da_1} S_r(a_0, a_1) \end{bmatrix} \xrightarrow{solve, a_0, a_1} [0.11766514898834059588 \quad 0.09609143373277995 4845]$$

a0: Slope a1: Slope

Again we have a successful bench. All values are in agreement.

Here's another function that extracts the local minimum value of any function. (Mathcad has one for the maximum value too)

$a_0 := 0$ $a_1 := 0$ You need arbitrary guess values for a0 and a1 for this one...

$$\text{minimize}(S_r, a_0, a_1) = \begin{bmatrix} 0.118 \\ 0.096 \end{bmatrix}$$ ***Still doing great!***

And finally a structure in Mathcad called a "Solve Block" which is rather popular with students since it can do a lot of different things.

We'll officially introduce you to this tool in Mathcad when in our next section on "Roots"

And with all of these methods, we get the same values!

Guess Values:
$a_0 := 0$ $a_1 := 0$

Constraints:
$$\frac{d}{da_0} S_r(a_0, a_1) = 0 \qquad \frac{d}{da_1} S_r(a_0, a_1) = 0$$

Solver:
$$\text{find}(a_0, a_1) = \begin{bmatrix} 0.118 \\ 0.096 \end{bmatrix}$$

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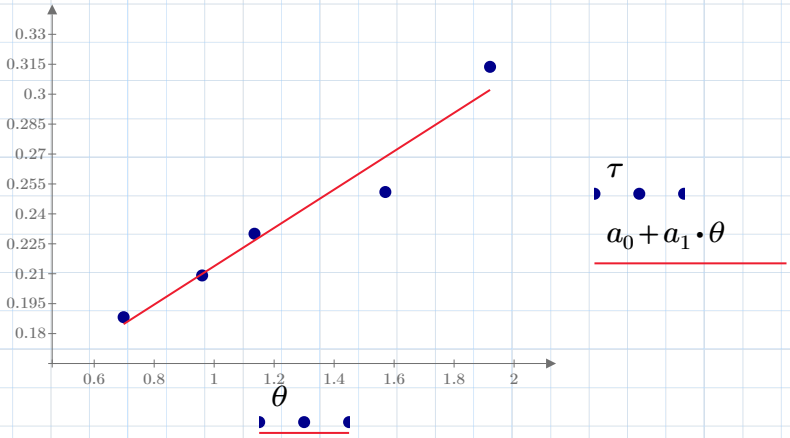
Now let's examine the quality of our regression.
Let's start by creating a new formula for our linear regression

$a_0 := \text{intercept}(\theta, \tau) = 0.118$ $a_1 := \text{slope}(\theta, \tau) = 0.096$ $\tau_\theta(\theta) := a_0 + a_1 \cdot \theta$

And it's always a good idea to plot things out....



Just by visual inspection you should expect a low RMSE and high correlations from the look-n-feel of this graph.

It makes a strong line through the data (with just one outlier that stands out)

The Total Sum of Squares (St or SST) is the baseline ***unskilled*** error and is the unskilled analog (i.e., equivalent) to the "***skilled***" Sum of the Squred Residuals (Sr or SSR). This is basically the varaince formula of your dependant variable (torque) without dividing by N

$S_t := \sum\left(\left(\tau - \tau_{mean}\right)^2\right) = 9.273 \cdot 10^{-3}$

And our Sr (our ***skilled*** error) is...

$S_r := \sum\left(\left(\tau - \tau_\theta(\theta)\right)^2\right) = 4.688 \cdot 10^{-4}$

Clearly we have an improvement here sicne Sr is notably less than St.
So let's articulate it with our other error metrics.
Our RMSE and Standard Error of the Estimate are...

$RMSE := \sqrt{\frac{S_r}{N}} = 9.683 \cdot 10^{-3}$ $s_{\tau\theta} := \sqrt{\frac{S_r}{N-2}} = 1.25 \cdot 10^{-2}$

And lets now create a basic baseline measure for skill where the error for a perfect forecast skill is zero. Remember that a good working definition of "*skill*" is how much better your method is to random chance or other *unskilled* method

$$Skill = \frac{yours - unskilled}{perfect - unskilled}$$

$skill := \frac{S_r - S_t}{0 - S_t} = 0.949$ $r2 := \frac{S_t - S_r}{S_t - 0} = 0.949$

And tying it to previous horseplay...

$\text{corr}(\theta, \tau) = 0.974$ $\text{corr}(\theta, \tau)^2 = 0.949$

So we now can officially link correlation with predictive skill!

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Now let's explore how to integrate confidence limits into our plots. The formual for a 95% confidence limit is is here:

$$\alpha := 100\% - 95\% = 0.05$$

$$CI95(\Theta) := \mathrm{qt}\left(1 - \frac{\alpha}{2}, N - 2\right) \cdot s_{\tau\theta} \cdot \sqrt{\frac{1}{N} + \frac{(\Theta - \theta_{mean})^2}{(N-1) \cdot {s_\theta}^2}}$$

Notice in the above formual I have two favors of "theta". The lowercase thetas are refering to the thetas in our original dataset. I am using the capital Theta for a "function variable" for any value of theta we chose to throw at it.

Now for the Prediction Interval - remember. You really should be wary of using this for original datasets that are not normally distributed. While we can do symetric CIs for the means thanks to the Central Limit Theorem we cannot do so for original data that is not a nice bell-curvy normal distribution.

$$PI95(\Theta) := \mathrm{qt}\left(1 - \frac{\alpha}{2}, N - 2\right) \cdot s_{\tau\theta} \cdot \sqrt{1 + \frac{1}{N} + \frac{(\Theta - \theta_{mean})^2}{(N-1) \cdot {s_\theta}^2}}$$

Let's all recall the structure of Confidence Limits by exploring math in the functions above.

We should have more certainty for a linear regression when we are in the center of the known data. As a result the confidence limits should be the thinnest there.

As we go outward into "here be dragons" territory, we will want to spread out those intervals. Likewise as we have greater net errors between our regression and our indivisual data points our CI (and PI) should once again fatten. If an "x" axis independant variable used to create the regression has a lower spread, we wil also see wider CI thicknesses as you aproach terra incognito.

Finally the more data we have to make a regression (or any other type of estimate) should also carry higher confidence and this make the regression confidence limits skinny.

And when plotted out, we get the chart to the right (remember that the Prediction Limits shown here are mostly demonstrative. Close inspection of the stats shows that we are NOT looking at normally-distributed data)